

# A key role of transversality condition in quantization of photon orbital angular momentum

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## Abstract

The effect of the constraint of transversality condition on the quantization of the photon orbital angular momentum is studied. From the point of view of quantum mechanics, the constraint expresses an entanglement between the intrinsic canonical variable, the polarization, and the extrinsic canonical variables. More importantly, its invariance under the rotation transformation of the vector wavefunction about the momentum turns out to mean the existence of degree of freedom of the Berry gauge, which appears as a constant unit vector. Because in each Berry-gauge representation, a two-component representation, the polarization is represented independently of the extrinsic canonical variables, the Berry-gauge degree of freedom has observable quantum effects. When the Berry-gauge degree of freedom of a paraxial beam is perpendicular to the propagation direction, the orbital angular momentum about the origin of the laboratory reference system reduces to its canonical part. Since the constraint together with the Schrödinger equation is equivalent to the Maxwell equations, the Berry-gauge degree of freedom reflects the relativistic effects of the photon in quantum mechanics.

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## I. INTRODUCTION

In their seminal work [1] Allen and his co-researchers introduced the notion of eigenstate of the optical orbital angular momentum (OAM), which is described by a phase factor  $\exp(il\phi)$  with  $l$  the eigenvalue. Since then a continuously growing number of theoretical and experimental works [2–12] appeared in the literature dealing with the eigenstate of the OAM at the level of single photons and its potential applications. It is well known [13] that the canonical quantization of the OAM  $\hat{\mathbf{L}}$  is based on the canonical commutation relation,

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k, \quad (1)$$

where Einstein's summation convention is assumed. This commutation relation in turn requires that the position  $\hat{\mathbf{X}}$  and momentum  $\hat{\mathbf{P}}$  satisfy the canonical commutation relations,

$$[\hat{X}_i, \hat{X}_j] = 0, \quad [\hat{P}_i, \hat{P}_j] = 0, \quad [\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}. \quad (2)$$

That is to say, the position needs to be commutative. Quantities  $\hat{\mathbf{X}}$  and  $\hat{\mathbf{P}}$  satisfying (2) are known as the canonical position and canonical momentum [14], respectively. They are called canonically conjugate [15]. However, being extremely relativistic, the photon is nonlocal in position space [16–19]. By this it is meant that the position of the photon cannot be commutative [20–25]. As a result, the OAM of the photon cannot be canonically quantized in accordance with the commutation relation (1). So how do we understand the above mentioned eigenvalue of the OAM?

Due to its nonlocality, the position-space wavefunction for the photon cannot be defined [26, 27] in the usual sense [13]. Only the momentum-space wavefunction can. In a formalism that is not manifestly relativistic [25], it is a vector function,  $\mathbf{f}(\mathbf{k}, t)$ , satisfying the Schrödinger equation

$$i\frac{\partial \mathbf{f}}{\partial t} = \omega \mathbf{f}, \quad (3)$$

where  $\mathbf{k}$  is the wavevector,  $\omega = ck$  is the angular frequency playing the role of the Hamiltonian, and  $k = |\mathbf{k}|$ . Here there is one peculiar feature that does not usually occur in quantum mechanics. This is that the vector wavefunction is constrained by the transversality condition

$$\mathbf{f} \cdot \mathbf{w} = 0, \quad (4)$$

where  $\mathbf{w} = \mathbf{k}/k$  is the unit wavevector. In the vector representation, the operator for the OAM about the origin is given by [25, 26, 28, 29]

$$\hat{\mathbf{L}} = -\hat{\mathbf{P}} \times \hat{\mathbf{X}}, \quad (5)$$

where

$$\hat{\mathbf{X}} = i\nabla_{\mathbf{k}}, \quad (6a)$$

$$\hat{\mathbf{P}} = \hbar\mathbf{k}, \quad (6b)$$

are the operators for the position and momentum, respectively, and  $\nabla_{\mathbf{k}}$  is the gradient operator with respect to  $\mathbf{k}$ . If the constraint (4) were absent, the position (6a) would be commutative and canonically conjugate to the momentum (6b).

From the point of view of quantum mechanics, the vector wavefunction as a multi-component function should describe the intrinsic variable of the photon. If this is the case, the constraint (4) means that the intrinsic variable is not independent of the momentum. They are entangled. The problem is what the intrinsic variable of the photon is. It is known [25, 26] that the Schrödinger equation (3) for the vector wavefunction together with the constraint (4) is equivalent to the free-space Maxwell equations. Denoted by  $\frac{1}{\sqrt{2}}(\mathbf{E} + \mathbf{E}^*)$  and  $\frac{1}{\sqrt{2}}(\mathbf{H} + \mathbf{H}^*)$ , respectively, the position-space electric and magnetic vectors that solve the free-space Maxwell equations are uniquely determined by the vector wavefunction in the following way,

$$\mathbf{E}(\mathbf{X}, t) = \frac{1}{(2\pi)^{3/2}} \int \left( \frac{\hbar\omega}{\varepsilon_0} \right)^{1/2} \mathbf{f} \exp(i\mathbf{k} \cdot \mathbf{X}) d^3k, \quad (7a)$$

$$\mathbf{H}(\mathbf{X}, t) = \frac{1}{(2\pi)^{3/2}} \int \left( \frac{\hbar\omega}{\mu_0} \right)^{1/2} \mathbf{w} \times \mathbf{f} \exp(i\mathbf{k} \cdot \mathbf{X}) d^3k. \quad (7b)$$

Because the electric and magnetic vectors are the physical entities that describe the polarization of the light [30], Eqs. (7) suggest that the intrinsic variable described by the vector wavefunction should be the polarization [26, 31]. Unfortunately, no polarization operator that shows entanglement with the momentum has been satisfactorily introduced. The main purpose of this paper is to investigate how the constraint (4) makes the polarization entangled with the momentum and how such an entanglement is related to the noncommutativity of the photon position.

For this purpose, we convert the vector representation into a representation in which no conditions such as Eq. (4) exist for the associated wavefunction. As is known, the constraint

(4) makes it possible to expand the vector wavefunction  $\mathbf{f}$  at each value of  $\mathbf{k}$  in terms of two orthogonal base vectors. Let be  $\mathbf{u}$  and  $\mathbf{v}$  a pair of mutually perpendicular unit vectors that form with  $\mathbf{w}$  a right-handed Cartesian system  $\mathbf{uvw}$  [32, 33], satisfying

$$\mathbf{u} \times \mathbf{v} = \mathbf{w}, \quad \mathbf{v} \times \mathbf{w} = \mathbf{u}, \quad \mathbf{w} \times \mathbf{u} = \mathbf{v}. \quad (8)$$

Choosing  $\mathbf{u}$  and  $\mathbf{v}$  as the base vectors as usual, we may write  $\mathbf{f}$  as

$$\mathbf{f} = f_{\mathbf{u}}\mathbf{u} + f_{\mathbf{v}}\mathbf{v}.$$

Putting the two expansion coefficients  $f_{\mathbf{u}}$  and  $f_{\mathbf{v}}$  together [34, 35] to form a two-component wavefunction  $\tilde{f} = \begin{pmatrix} f_{\mathbf{u}} \\ f_{\mathbf{v}} \end{pmatrix}$ , we can rewrite  $\mathbf{f}$  as

$$\mathbf{f} = \varpi \tilde{f}, \quad (9)$$

where  $\varpi = (\mathbf{u} \ \mathbf{v})$  is a 3-by-2 matrix consisting of the two base vectors and vectors of three components such as  $\mathbf{u}$  and  $\mathbf{v}$  are expressed as column matrices. Since the matrix  $\varpi$  guarantees that the constraint (4) on the vector wavefunction (9) is satisfied, no such conditions exist for the two-component wavefunction. But for a given vector wavefunction, the two-component wavefunction is indefinite because Eqs. (8) cannot completely determine the base vectors up to a rotation about the wavevector [33]. To get a definite two-component wavefunction, it is required to manage to fix the base vectors. This is usually done in classical theory [32, 36, 37] by introducing a constant unit vector, denoted by  $\mathbf{I}$ , as follows,

$$\mathbf{u} = \mathbf{v} \times \frac{\mathbf{k}}{k}, \quad \mathbf{v} = \frac{\mathbf{I} \times \mathbf{k}}{|\mathbf{I} \times \mathbf{k}|}. \quad (10)$$

Unexpectedly, so introduced unit vector turns out in quantum mechanics to be a Berry-gauge degree of freedom (the meaning of which will be explained in Section IV) so that the two-component representation denoted by this unit vector is a Berry-gauge representation. Here are the main results.

The Berry-gauge degree of freedom fixes, through Eqs. (10), the local reference system  $\mathbf{uvw}$  relative to which the polarization is canonically represented by the Pauli matrices in the Berry-gauge representation. By this it is meant that the Berry-gauge degree of freedom determines the entanglement between the polarization and momentum in such a way that the polarization is represented independently of the momentum in the Berry-gauge representation. As a result, only in a particular Berry gauge can the momentum be

canonical. The conjugate canonical position is no longer the position of the photon in the laboratory reference system. It is instead the position of the photon relative to a reference point that is determined by the Berry-gauge potential. The OAM about that reference point is a canonical OAM satisfying the canonical commutation relation (1). Because quantum numbers depend only on commuting canonical variables, the Berry-gauge degree of freedom has observable quantum effects. A comparison between the OAM about the origin of the laboratory reference system and the canonical OAM reveals that the so-called eigenvalue of the OAM is actually the eigenvalue of the canonical OAM in the case in which the Berry-gauge degree of freedom of a paraxial beam is perpendicular to its propagation direction.

## II. INTRODUCTION OF TWO-COMPONENT REPRESENTATION

The one-to-one correspondence between the vector wavefunction and the electric and magnetic vectors indicates that each vector wavefunction can describe a particular photon state. To explore the role of the constraint (4) in quantum mechanics, we try to convert the vector representation into a two-component representation in which the wavefunction is free of such conditions.

### A. From constraint to two-component wavefunction

We have changed the constraint (4) into the matrix  $\varpi$  that expresses the vector wavefunction in terms of a two-component entity via Eq. (9). It performs a quasi unitary transformation in the following sense. On one hand,  $\varpi$  acts on the two-component entity to give a vector wavefunction that satisfies the constraint (4). It is easy to prove that

$$\varpi^\dagger \varpi = I_2, \quad (11)$$

where  $I_2$  is the 2-by-2 unit matrix and the superscript  $\dagger$  stands for the conjugate transpose. On the other hand, multiplying both sides of Eq. (9) by  $\varpi^\dagger$  from the left and using Eq. (11), we get

$$\tilde{f} = \varpi^\dagger \mathbf{f}. \quad (12)$$

It says that  $\varpi^\dagger$  acts on a vector wavefunction to give a two-component entity. A straightforward calculation yields  $\varpi \varpi^\dagger = I_3 - \mathbf{w} \mathbf{w}^\dagger$ , where  $I_3$  is the 3-by-3 unit matrix. But when

the constraint (4) is considered, we have

$$(\varpi\varpi^\dagger)\mathbf{f} = \mathbf{f}.$$

Keeping in mind that  $\varpi^\dagger$  always acts on the vector wavefunction  $\mathbf{f}$ , we may rewrite it simply as

$$\varpi\varpi^\dagger = I_3. \quad (13)$$

Eqs. (11) and (13) express the quasi unitarity [38] of the transformation matrix  $\varpi$ .  $\varpi^\dagger$  is the Moore-Penrose pseudo inverse of  $\varpi$ , and vice versa.

From Eq. (13) it follows that

$$\tilde{f}^\dagger \tilde{f} = \mathbf{f}^\dagger \mathbf{f},$$

which tells that the two-component entity appears as a different kind of momentum-space wavefunction. Now that the matrix  $\varpi$  guarantees that the vector wavefunction (9) satisfies the constraint (4), the two-component wavefunction will not be subject to such conditions. Multiplying both sides of Eq. (3) by  $\varpi^\dagger$  from the left and making use of Eq. (12), we arrive at the following Schrödinger equation for the two-component wavefunction,

$$i\frac{\partial \tilde{f}}{\partial t} = \omega \tilde{f}, \quad (14)$$

which is the same as the Schrödinger equation (3) for the vector wavefunction.

## B. A constant unit vector to denote the two-component representation

But, as mentioned before, to get a definite two-component wavefunction from a given vector wavefunction, we have to introduce a constant unit vector  $\mathbf{I}$  to fix the quasi unitary matrix  $\varpi$  by Eqs. (10). Let us see how the two-component wavefunction depends on the choice of the constant unit vector.

To do this, we choose a different unit vector,  $\mathbf{I}'$  say, to fix the base vectors,

$$\mathbf{u}' = \mathbf{v}' \times \frac{\mathbf{k}}{k}, \quad \mathbf{v}' = \frac{\mathbf{I}' \times \mathbf{k}}{|\mathbf{I}' \times \mathbf{k}|}. \quad (15)$$

In this case, the two-component wavefunction for the same vector wavefunction  $\mathbf{f}$  is given by

$$\tilde{f}' = \varpi'^\dagger \mathbf{f}, \quad (16)$$

where  $\varpi' = (\mathbf{u}' \ \mathbf{v}')$ . As remarked earlier, the new base vectors  $\mathbf{u}'$  and  $\mathbf{v}'$  are related to the old ones  $\mathbf{u}$  and  $\mathbf{v}$  by a rotation about  $\mathbf{k}$ . Letting be  $\Phi(\mathbf{I}, \mathbf{I}'; \mathbf{k})$  the  $\mathbf{k}$ -dependent rotation angle, such a rotation can be expressed compactly as

$$\varpi' = \exp[-i(\hat{\Sigma} \cdot \mathbf{w})\Phi]\varpi, \quad (17)$$

where  $(\hat{\Sigma}_k)_{ij} = -i\epsilon_{ijk}$  with  $\epsilon_{ijk}$  the Levi-Civita pseudotensor. Eq. (17) can also be rewritten as [39]

$$\varpi' = \varpi \exp(-i\hat{\sigma}_3\Phi) \quad (18)$$

in terms of the Pauli matrix

$$\hat{\sigma}_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

Substituting Eq. (18) into Eq. (16) and noticing Eq. (12), we find

$$\tilde{f}' = \exp(i\hat{\sigma}_3\Phi)\tilde{f}. \quad (19)$$

It is pointed out that the rotation angle  $\Phi$  is determined only by the change of the unit vector  $\mathbf{I}$ , having nothing to do with the vector wavefunction.

However, given a unit vector  $\mathbf{I}$ , the quasi unitarity of the matrix  $\varpi$  ensures that the two-component wavefunction has a one-to-one correspondence with the vector wavefunction via Eq. (12). This shows that the unit vector to fix the quasi unitary matrix  $\varpi$  denotes a two-component representation by Eq. (12). From this result it is concluded that a two-component wavefunction, though not constrained by conditions such as Eq. (4), is physically meaningful only when considered in a particular representation. In the following we will gradually analyze the physical significance of the fact that the unit vector  $\mathbf{I}$  denotes a two-component representation.

### III. INDEPENDENT REPRESENTATION OF THE POLARIZATION

We will show in this section that the unit vector  $\mathbf{I}$  determines the entanglement between the polarization and momentum in such a way that they can be represented independently of each other in the corresponding two-component representation. It was pointed out a long time ago by Darwin [40] that the polarization of the photon cannot be completely described by the spin. But how the polarization differs from the spin still remains unclear [41, 42]. So

before discussing the entanglement of the polarization with the momentum, it is beneficial to distinguish the polarization from the spin. To this end, we first consider the spin operator in the two-component representation.

### A. Spin operator in the two-component representation

The spin operator in the vector representation takes the form [25, 26, 28, 29]  $\hat{\mathbf{S}} = \hbar \hat{\boldsymbol{\Sigma}}$ . According to the quasi unitary transformation (12), the spin operator in the two-component representation is given by

$$\hat{\mathbf{s}} = \hbar \varpi^\dagger \hat{\boldsymbol{\Sigma}} \varpi.$$

Upon decomposing the vector operator  $\hat{\boldsymbol{\Sigma}}$  in the local reference system  $\mathbf{uvw}$  as

$$\hat{\boldsymbol{\Sigma}} = (\hat{\boldsymbol{\Sigma}} \cdot \mathbf{u})\mathbf{u} + (\hat{\boldsymbol{\Sigma}} \cdot \mathbf{v})\mathbf{v} + (\hat{\boldsymbol{\Sigma}} \cdot \mathbf{w})\mathbf{w}$$

and taking Eqs. (8) into account, we find

$$\hat{\mathbf{s}} = \hbar \hat{\sigma}_3 \mathbf{w}, \tag{20}$$

where

$$\hat{\sigma}_3 = \varpi^\dagger (\hat{\boldsymbol{\Sigma}} \cdot \mathbf{w}) \varpi \tag{21}$$

is the Pauli matrix (18). Here we arrive in a simple way at the well-known conclusion that the spin of the photon lies entirely on its propagation direction. The Pauli matrix  $\hat{\sigma}_3$  represents essentially the magnitude of the spin, known as the helicity. As a result, the Cartesian components of the spin commute,

$$[\hat{s}_i, \hat{s}_j] = 0.$$

This is what van Enk and Nienhuis obtained in a second-quantization framework [43, 44].

It is noticed that the spin operator (20) in the two-component representation does not depend on the unit vector  $\mathbf{I}$ . By this it is meant that the two-component wavefunction is itself sufficient to determine the spin, no matter which representation it belongs to. Considering that the two-component wavefunction is physically meaningful only when considered in a particular representation, it is expected that the unit vector denoting the two-component representation will play a key role in distinguishing the polarization from the spin.



To demonstrate this, it is proper to consider two photon states that are described by the same two-component wavefunction  $\tilde{f}$  but in two different representations. One is described in the representation  $\mathbf{I}$ , having the vector wavefunction (9). The other is in the representation  $\mathbf{I}'$  and has the following vector wavefunction,

$$\mathbf{f}' = \varpi' \tilde{f}, \quad (22)$$

which is related to the vector wavefunction (9) via

$$\mathbf{f}' = \exp[-i(\hat{\Sigma} \cdot \mathbf{w})\Phi]\mathbf{f}, \quad (23)$$

by virtue of Eq. (17). Eq. (23) describes a rotation transformation on the vector wavefunction about the momentum. It is no doubt that these two states have the same spin. But they cannot have the same polarization in the light of Eqs. (7). To see this more clearly, we need to know how to represent the polarization in the two-component representation.

## B. Polarization operator in the two-component representation

It is well known [15] that a two-component wavefunction  $\tilde{f}$  must be an eigenfunction of the density matrix of the following form, having eigenvalue 1,

$$\hat{\rho} = \frac{1}{2}(1 + \mathbf{s} \cdot \hat{\boldsymbol{\zeta}}),$$

where

$$\mathbf{s} = \frac{\tilde{f}^\dagger \hat{\boldsymbol{\zeta}} \tilde{f}}{\tilde{f}^\dagger \tilde{f}} \quad (24)$$

and  $\hat{\boldsymbol{\zeta}}$  is a vector operator consisting of the Pauli matrices. Because the vector (24) is known in quantum mechanics as the polarization, the vector operator  $\hat{\boldsymbol{\zeta}}$  should be the polarization operator in the two-component representation. Our aim here is to analyze how it depends on the unit vector  $\mathbf{I}$ .

The constraint (4) requires that the vector wavefunction  $\mathbf{f}$  at each value of  $\mathbf{k}$  is located in the plane normal to  $\mathbf{k}$ . So the two components of the wavefunction (12) are the projection of  $\mathbf{f}$  on the transverse axes,  $\mathbf{u}$  and  $\mathbf{v}$ , of the local reference system  $\mathbf{uvw}$ . For a plane-wave state in position space, the two-component wavefunction is essentially the quantum-mechanical analogue of the Jones vector in classical optics. Based on the classical description of the

polarization of the plane wave [30, 45], it is justified to write the polarization operator in the two-component representation as

$$\hat{\boldsymbol{\zeta}} = \hat{\sigma}_1 \mathbf{u} + \hat{\sigma}_2 \mathbf{v} + \hat{\sigma}_3 \mathbf{w} \quad (25)$$

in terms of the Pauli matrices,

$$\hat{\sigma}_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{\sigma}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (26)$$

That is to say, the wavefunction in any two-component representation describes the polarization of the photon in such a way that the Pauli matrices (26) represent the Cartesian components of the polarization in the local reference system  $\mathbf{uvw}$  that is fixed by the corresponding unit vector  $\mathbf{I}$ . In view of this, the unit vector that denotes the two-component representation plays the role of determining the entanglement of the polarization with the momentum via Eq. (25). In the remainder of this paper, we will refer only to the vector (24) as the polarization. Substituting Eq. (25) into Eq. (24) gives

$$\mathbf{s} = s_1 \mathbf{u} + s_2 \mathbf{v} + s_3 \mathbf{w}, \quad (27)$$

where

$$s_i = \frac{\tilde{f}^\dagger \hat{\sigma}_i \tilde{f}}{\tilde{f}^\dagger \tilde{f}}.$$

With the definition (24), it is straightforward to compare the polarization of the two states (9) and (22). As stated, they are described in different two-component representations by the same wavefunction. The former is described in the representation  $\mathbf{I}$  and therefore has the polarization (27). The latter is described in the representation  $\mathbf{I}'$ . The polarization operator in this case reads

$$\hat{\boldsymbol{\zeta}}' = \hat{\sigma}_1 \mathbf{u}' + \hat{\sigma}_2 \mathbf{v}' + \hat{\sigma}_3 \mathbf{w}, \quad (28)$$

where  $\mathbf{u}'$  and  $\mathbf{v}'$  are given by Eqs. (15). Accordingly, the polarization is given by

$$\mathbf{s}' = s_1 \mathbf{u}' + s_2 \mathbf{v}' + s_3 \mathbf{w}.$$

Upon taking Eq. (17) into account, we finally have

$$\mathbf{s}' = \exp[-i(\hat{\boldsymbol{\Sigma}} \cdot \mathbf{w})\Phi] \mathbf{s}, \quad (29)$$

which is in perfect agreement with the relation (23) between the two vector wavefunctions.

The difference between the spin and polarization is now clear. It is seen from Eqs. (20) and (25) that the former is just the longitudinal part of the latter. That is to say, the helicity is the longitudinal component of the polarization. More importantly, because the Pauli matrices satisfy the canonical commutation relation of the angular momentum,

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k,$$

except for a factor two, the polarization represented this way can be viewed as a canonical variable, called the intrinsic canonical variable.

### C. Independence of the polarization in the two-component representation

We have now identified the polarization operator (25) in the two-component representation. Since the unit vectors  $\mathbf{u}$ ,  $\mathbf{v}$ , and  $\mathbf{w}$  denote the Cartesian axes of the local reference system that is fixed by the unit vector  $\mathbf{I}$ , it follows that the polarization of the photon can be completely represented by the constant Pauli matrices (26) in the two-component representation. Observing that the momentum operator in the two-component representation remains the same as in the vector representation,

$$\hat{\mathbf{p}} = \varpi^\dagger \hat{\mathbf{P}} \varpi = \hbar \mathbf{k}, \quad (30)$$

in accordance with the quasi unitary transformation (12), so represented polarization is independent of the momentum. By this it is meant that a constant two-component wavefunction describes, according to Eq. (27), a polarization the components of which in the local reference system  $\mathbf{uvw}$  are constant. One example is the eigenfunction of the helicity  $\hat{\sigma}_3$  with eigenvalue  $\sigma = \pm 1$ ,

$$\tilde{\alpha}_\sigma = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i\sigma \end{pmatrix}. \quad (31)$$

Obviously, it describes the polarization  $\mathbf{s} = \sigma \mathbf{w}$ .

Nevertheless, it should be emphasized that such an independence does not mean the disentanglement of the polarization from the momentum. The key point is what determines the entanglement between the polarization and momentum is the unit vector that denotes the two-component representation. After all, the polarization operator (25) as a whole depends on the unit vectors of the Cartesian axes of the local reference system  $\mathbf{uvw}$ .

#### IV. BERRY GAUGE AND CANONICAL POSITION

We have seen in preceding section that the polarization and momentum are so entangled that they can be independently represented in any two-component representation. The reason is that the constant unit vector denoting the two-component representation is a Berry-gauge degree of freedom, which is the topic of this section. We will see that the Berry-gauge degree of freedom determines, through the Berry-gauge potential, a reference point relative to which the position of the photon is canonical.

##### A. Identification of the canonical position

According to Eq. (12), the position operator in the two-component representation is transformed from Eq. (6a) as follows,

$$\hat{\mathbf{x}} = \varpi^\dagger \hat{\mathbf{X}} \varpi = \hat{\boldsymbol{\xi}} + \hat{\mathbf{b}}, \quad (32)$$

which splits two parts:

$$\hat{\boldsymbol{\xi}} = i\nabla_{\mathbf{k}}, \quad (33a)$$

$$\hat{\mathbf{b}} = i\varpi^\dagger (\nabla_{\mathbf{k}} \varpi). \quad (33b)$$

The first part (33a) has the same form as the position operator (6a) in the vector representation. But because no conditions such as Eq. (4) exist for the two-component wavefunction, it is commutative,

$$[\hat{\xi}_i, \hat{\xi}_j] = 0, \quad (34)$$

the same as the momentum operator (30),

$$[\hat{p}_i, \hat{p}_j] = 0. \quad (35)$$

It has the following commutation relation with the momentum,

$$[\hat{\xi}_i, \hat{p}_j] = i\hbar\delta_{ij}. \quad (36)$$

The second part (33b) is solely determined by the matrix  $\varpi$ . A straightforward calculation gives

$$\hat{\mathbf{b}} = \hat{\sigma}_3 \mathbf{A}, \quad (37)$$

where  $\hat{\sigma}_3$  is the helicity operator and

$$\mathbf{A}(\mathbf{I}, \mathbf{k}) = \frac{\mathbf{I} \cdot \mathbf{k}}{k|\mathbf{I} \times \mathbf{k}|} \mathbf{v}. \quad (38)$$

Commuting with the Hamiltonian, this part represents a constant of motion. Moreover, its Cartesian components also commute,

$$[\hat{b}_i, \hat{b}_j] = 0. \quad (39)$$

With the help of Eqs. (34) and (39), it is not difficult to find

$$[\hat{x}_i, \hat{x}_j] = i\hat{\sigma}_3 \epsilon_{ijk} B_k, \quad (40)$$

where

$$\mathbf{B} = \nabla_{\mathbf{k}} \times \mathbf{A} = -\frac{\mathbf{w}}{k^2}, \quad \mathbf{w} \neq \pm \mathbf{I}. \quad (41)$$

This shows that the constraint (4) on the vector wavefunction does reflect the noncommutativity of the position. These results are explained as follows.

Eqs. (34)-(36) are nothing but the canonical commutation relations between  $\hat{\boldsymbol{\xi}}$ , the first part of  $\hat{\mathbf{x}}$ , and  $\hat{\mathbf{p}}$ . So the operator  $\hat{\boldsymbol{\xi}}$  represents such a position  $\boldsymbol{\xi}$  that is canonically conjugate to the momentum, called the canonical position. Accordingly, the operator  $\hat{\mathbf{b}}$ , the second part of  $\hat{\mathbf{x}}$ , represents a reference point relative to which the canonical position is measured. It is seen from Eq. (37) that this is a point that depends on the unit vector  $\mathbf{I}$  through the vector function  $\mathbf{A}$ . For comparison, the position  $\mathbf{X}$  that is represented by the operator  $\hat{\mathbf{x}}$  itself will be called the laboratory position. To understand the commutation relation (40) of the laboratory position, it is essential to explore the meaning of  $\mathbf{A}$  and its  $\mathbf{I}$ -dependence.

## B. The degree of freedom for the Berry gauge

Substituting Eq. (37) into Eq. (32), we have

$$\hat{\mathbf{x}} = \hat{\boldsymbol{\xi}} + \hat{\sigma}_3 \mathbf{A}. \quad (42)$$

If the laboratory position  $\hat{\mathbf{x}}$  is regarded as the analog of the kinetic momentum of an electrically charged particle in a magnetic field and the canonical position  $\hat{\boldsymbol{\xi}}$  is regarded as the analog of the canonical momentum of the particle [46], then the helicity  $\hat{\sigma}_3$  can be regarded as the analog of the electric charge of the particle and the vector function  $\mathbf{A}$  can be regarded

as the analog of the vector potential of the magnetic field. That is,  $\mathbf{A}$  appears as the gauge potential of the gauge field (41). Indeed, the commutation relation (40) of the laboratory position that depends on the gauge field (41) is analogous to the commutation relation of the kinetic momentum of the charged particle that depends on the magnetic field.

Furthermore, consider a different two-component representation  $\mathbf{I}'$ . The operator in this case for the laboratory position becomes

$$\hat{\mathbf{x}}' = \varpi'^{\dagger} \hat{\mathbf{X}} \varpi' = \hat{\boldsymbol{\xi}} + \hat{\mathbf{b}}',$$

where

$$\hat{\mathbf{b}}' = \hat{\sigma}_3 \mathbf{A}' \quad (43)$$

and  $\mathbf{A}' = \mathbf{A}(\mathbf{I}', \mathbf{k})$ . In addition, from Eq. (33b) it follows that  $\hat{\mathbf{b}}' = i\varpi'^{\dagger}(\nabla_{\mathbf{k}}\varpi')$ . With the help of Eqs. (18) and (11), we get

$$\hat{\mathbf{b}}' = \hat{\mathbf{b}} + \hat{\sigma}_3 \nabla_{\mathbf{k}} \Phi. \quad (44)$$

A comparison of Eqs. (43) and (37) gives

$$\mathbf{A}' = \mathbf{A} + \nabla_{\mathbf{k}} \Phi, \quad (45)$$

indicating that under the change of  $\mathbf{I}$ , the gauge potential undergoes a gauge transformation with  $\Phi$  the corresponding gauge function. This shows that the unit vector  $\mathbf{I}$  is a kind of gauge degree of freedom. The meaning of it is explained as follows.

The gauge field (41) corresponding to the gauge potential (38) is a Berry-gauge field [47] that is produced by a magnetic monopole [48] of unit strength in momentum space [49, 50]. The gauge degree of freedom  $\mathbf{I}$ , called the Berry-gauge degree of freedom, indicates the orientation of the monopole's Dirac string. The gauge transformation (45) serves to reorient the Dirac string from  $\mathbf{I}$  to  $\mathbf{I}'$  and is thus a singular transformation [51]. In a word, each unit vector  $\mathbf{I}$  represents a particular Berry gauge that is expressed by the Berry-gauge potential (38). On this basis, the two-component representation denoted by the Berry-gauge degree of freedom is a Berry-gauge representation. And Eq. (19) is the gauge transformation on the two-component wavefunction that corresponds to the gauge transformation (45) on the Berry-gauge potential. These results lead us to an unusual conclusion that the commutation relation (40) of the laboratory position is dependent on the Berry gauge.

## V. PHYSICAL SIGNIFICANCE OF THE BERRY GAUGE

The same as the dependence of the local reference system  $\mathbf{uvw}$  on the momentum embodies the entanglement of the polarization with the momentum, the dependence of the reference point (37) on the helicity embodies the entanglement of the helicity with the canonical position. The dependence of the reference point (37) on the Berry-gauge potential indicates that the entanglement between the helicity and canonical position is determined by the Berry-gauge degree of freedom, the same as the entanglement between the polarization and canonical momentum. In a word, each Berry gauge determines a particular way in which the intrinsic canonical variable, the polarization, is entangled with the extrinsic canonical variables such as the canonical position and canonical momentum. This means that the canonical variables, including the intrinsic and extrinsic, have to be associated with a particular Berry gauge.

But Eq. (33a) shows that the canonical position is represented independently of the polarization in the Berry-gauge representation, the same as the canonical momentum. That is to say, the Berry-gauge representation is such a representation in which the extrinsic canonical variables are represented independently of the intrinsic canonical variable. This is a quantum-mechanical formalism that we are familiar with. Since the quantum numbers specifying an eigenstate depend only on commuting canonical variables, the Berry-gauge degree of freedom would have its peculiar quantum effects. We have shown in preceding section that the same two-component wavefunction in different Berry gauge describes different state of polarization, which is physically observable. At the end of this section we present another observable effect, the dependence of the barycenter on the Berry-gauge degree of freedom.

Since the helicity and canonical momentum are both constants of motion, we consider one of their simultaneous eigenstates, the wavefunction of which in the Berry-gauge representation is given by

$$\tilde{f}_{\sigma, \mathbf{k}_0} = \tilde{\alpha}_{\sigma} \delta^3(\mathbf{k} - \mathbf{k}_0) \exp(-i\omega t), \quad (46)$$

where  $\tilde{\alpha}_{\sigma}$  is the eigenfunction (31) of the helicity operator  $\hat{\sigma}_3$  and  $\mathbf{k}_0$  is the eigenvalue of the canonical momentum. This is a plane-wave state in position space. Substituting Eq. (46) into Eq. (9) gives for its wavefunction in the vector representation,

$$\mathbf{f}_{\sigma, \mathbf{k}_0; \mathbf{I}} = \mathbf{a}_{\sigma, \mathbf{k}; \mathbf{I}} \delta^3(\mathbf{k} - \mathbf{k}_0) \exp(-i\omega t), \quad (47)$$

where

$$\mathbf{a}_{\sigma,\mathbf{k};\mathbf{I}} = \varpi \tilde{\alpha}_{\sigma} = \frac{1}{\sqrt{2}}(\mathbf{u} + i\sigma\mathbf{v}) \quad (48)$$

is the eigenfunction of the helicity operator in the vector representation,  $\hat{\Sigma} \cdot \mathbf{w}$ . Furthermore, substituting Eq. (47) into Eq. (7a) gives for its electric vector in position space,

$$\mathbf{E}_{\sigma,\mathbf{k}_0;\mathbf{I}} = \frac{1}{2\pi} \left( \frac{\hbar\omega_0}{2\pi\varepsilon_0} \right)^{1/2} \mathbf{a}_{\sigma,\mathbf{k}_0;\mathbf{I}} \exp[i(\mathbf{k}_0 \cdot \mathbf{X} - \omega_0 t)],$$

where  $\omega_0 = ck_0$  and  $k_0 = |\mathbf{k}_0|$ . It is clear that in order to determine such an eigenstate, we need not only the eigenvalues of the helicity and canonical momentum but also the Berry-gauge degree of freedom! To appreciate the effect of the Berry-gauge degree of freedom, it is only necessary to remind that the wavefunction (46) describes the eigenstate of the operator (37) with the eigenvalue,

$$\mathbf{b}_{\sigma,\mathbf{k}_0;\mathbf{I}} = \sigma \frac{\mathbf{I} \cdot \mathbf{k}_0}{k_0 |\mathbf{I} \times \mathbf{k}_0|^2} \mathbf{I} \times \mathbf{k}_0. \quad (49)$$

Observing that the expectation value of the canonical position in this state vanishes,  $\langle \hat{\xi} \rangle = 0$ , the eigenvalue (49) is nothing but the barycenter of the photon in the sense that it is equal to the expectation value of the laboratory position,  $\langle \hat{\mathbf{x}} \rangle = \mathbf{b}_{\sigma,\mathbf{k}_0;\mathbf{I}}$ . It illustrates that the same set of quantum numbers  $\{\sigma, \mathbf{k}_0\}$  in different Berry gauge stands for different eigenstate, having different barycenter. What deserves emphasizing here is that the helicity has crucial contribution to the barycenter. This is why the so-called spin Hall effect of light [52, 53] can be quantitatively explained by the change of the Berry-gauge degree of freedom [54].

## VI. INTERPRETATION OF THE EIGENVALUE OF THE OAM

Now we are ready to deal with the OAM. The same as the position operator (32), the operator in the Berry-gauge representation for the OAM about the origin of the laboratory reference system also splits into two parts,

$$\hat{\mathbf{l}} = \varpi^\dagger \hat{\mathbf{L}} \varpi = \hat{\boldsymbol{\lambda}} + \hat{\mathbf{m}}. \quad (50)$$

The first part

$$\hat{\boldsymbol{\lambda}} = -\hat{\mathbf{p}} \times \hat{\boldsymbol{\xi}} \quad (51)$$

represents the OAM of the photon about the barycenter. Thanks to the canonical commutation relations (34)-(36), it satisfies the canonical commutation relation of the angular



momentum,

$$[\hat{\lambda}_i, \hat{\lambda}_j] = i\hbar\epsilon_{ijk}\hat{\lambda}_k, \quad (52)$$

and will be referred to as the canonical OAM. Clearly, it is a constant of motion,

$$[\hat{\boldsymbol{\lambda}}, \omega] = 0. \quad (53)$$

The second part

$$\hat{\mathbf{m}} \equiv \hat{\mathbf{b}} \times \hat{\mathbf{p}} = \hbar\hat{\sigma}_3 \frac{\mathbf{I} \cdot \mathbf{k}}{|\mathbf{I} \times \mathbf{k}|} \mathbf{u} \quad (54)$$

represents the OAM of the photon concentrated at the barycenter. Different from the first part, its Cartesian components commute,

$$[\hat{m}_i, \hat{m}_j] = 0. \quad (55)$$

But the same as the first part, it is a constant of motion,

$$[\hat{\mathbf{m}}, \omega] = 0. \quad (56)$$

As a result of Eqs. (53) and (56), the total OAM is a constant of motion, too.

It is interesting to note that the expression (50) for the total OAM can find its counterpart in classical mechanics [55]: the angular momentum of a system about a reference point is the angular momentum of the system concentrated at the barycenter plus the angular momentum of the system about the barycenter. With the help of Eqs. (52) and (55), it is not difficult to find for the commutation relation of the total OAM,

$$[\hat{l}_i, \hat{l}_j] = i\hbar\epsilon_{ijk}(\hat{l}_k - \hat{s}_k), \quad (57)$$

in agreement with what van Enk and Nienhuis obtained in a second-quantization framework [43, 44]. This shows that the total OAM cannot be canonically quantized. Only its first part, the canonical OAM, can. In addition, the dependence of the second part on the helicity explains why the total angular momentum of a non-paraxial beam cannot be separated into helicity-independent OAM and helicity-dependent spin [56].

A paraxial light beam is a photon state in which all the plane-wave component travels in almost the same direction, the propagation axis. If the Berry-gauge degree of freedom of a paraxial beam is perpendicular to the propagation axis, it follows from Eq. (54) that  $\hat{\mathbf{m}} \approx 0$ . In this case, the total OAM is approximately the canonical OAM,  $\hat{\mathbf{l}} \approx \hat{\boldsymbol{\lambda}}$ . The paraxial beam that was discussed by Allen et. al. [1] is just such a beam [28]. The so-called eigenvalue of the OAM is actually the eigenvalue of the canonical OAM.

## VII. CONCLUSIONS AND COMMENTS

In conclusion, it is revealed that the invariance of the constraint (4) under the transformation (23) on the vector wavefunction means the existence of degree of freedom of the Berry gauge. What is important is that in any Berry gauge the intrinsic canonical variable can be represented independently of the extrinsic canonical variables. From this result it is inferred that only in a particular Berry gauge can the radiation field be canonically quantized.

It is noted that the Schrödinger equation (14) for the two-component wavefunction in a particular Berry-gauge representation is not relativistic. This is different from the Schrödinger equation (3) for the vector wavefunction. Even though it is not manifestly relativistic, Eq. (3) together with the constraint (4) is equivalent to the free-space Maxwell equations [25, 26], which are relativistic. In fact, Pryce [20] once recast the free-space Maxwell equations into two relativistic quantum-mechanical equations. From this point of view, the Berry-gauge degree of freedom may be regarded as the reflection of the relativistic effects of the photon in quantum mechanics.

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